

# The Moyal Equation for open quantum systems

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We generalize the Moyal equation, which describes the dynamics of quantum observables in phase space, to quantum systems coupled to a reservoir. It is shown that phase space observables become functionals of fluctuating noise forces introduced by the coupling to the reservoir. For Markovian reservoirs, the Moyal equation turns into a functional differential equation in which the reservoir's effect can be described by a single parameter.

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## I. INTRODUCTION

In the study of quantum systems, researchers employ different methods to achieve their goals. For instance, the dynamics of a system can be described using the Schrödinger equation for a state or the Heisenberg equation for operators. Another example is to use the Wigner function  $W(q, p)$  to describe the state by a function in phase space rather than by a wavefunction  $\psi(q)$  or a density matrix  $\hat{\rho}$ .

The Wigner function [1, 2], which for a one-dimensional system takes the form

$$W(q, p) = \frac{1}{2\pi\hbar} S[\hat{\rho}](q, p) \quad (1)$$

$$S[\hat{\rho}](q, p) = \int dq' \langle q + \frac{1}{2}q' | \hat{\rho} | q - \frac{1}{2}q' \rangle e^{-iq'p/\hbar}, \quad (2)$$

has become a very popular tool to visualize the state of a quantum system and to compare it to classical systems. To evaluate mean values of observables  $\hat{A}$  in phase space one needs to introduce Weyl symbols  $S[\hat{A}](q, p)$ , which represent operators on Hilbert space by functions on phase space [3, 4]. To keep the notation concise we will write  $A(q, p)$  instead  $S[\hat{A}](q, p)$ , i.e., the symbol has the same notation as the operator but without a hat.

The dynamics of the Wigner function is described by  $\partial_t W = \{H, W\}_M$ , where  $H$  is the Weyl symbol of the Hamiltonian. The Moyal bracket of two Weyl symbols  $A, B$  is defined as [5–8]

$$\{A, B\}_M = \frac{1}{i\hbar} (A \star B - B \star A). \quad (3)$$

The star product  $\star$  between two symbols is a representation of the non-commutative product between operators in phase space [9–13]. For our purpose it can be written as

$$A(q, p) \star B(q, p) = A(\mathcal{L})B(q, p) = B(\mathcal{R})A(q, p) \quad (4)$$

$$A(\mathcal{L}) = A\left(q + i\frac{\hbar}{2}\partial_p, p - i\frac{\hbar}{2}\partial_q\right) \quad (5)$$

$$B(\mathcal{R}) = B\left(q - i\frac{\hbar}{2}\partial_p, p + i\frac{\hbar}{2}\partial_q\right). \quad (6)$$

In the limit  $\hbar \rightarrow 0$ , the Moyal bracket turns into the classical Poisson bracket and the dynamics of the Wigner function is described by the Liouville equation [5].

The dynamical equation for the Wigner function is the analogue of the Schrödinger equation in phase space. Likewise, the analogue of the Heisenberg equation of motion for operators  $\hat{A}$  is the Moyal equation

$$\partial_t A = \{A, H\}_M. \quad (7)$$

By combining the two possibilities (Hilbert space and phase space) to represent a quantum system with the two possibilities to describe its dynamics (Schrödinger picture and Heisenberg picture), we thus arrive at four different ways to study its evolution.

The dynamical equations above apply to perfectly isolated quantum systems. However, for a realistic description of experiments, the coupling to the environment has to be taken into account. This is accomplished by considering open quantum systems [14, 15], where the system of interest is coupled to another system (the reservoir) that cannot be accessed in an experiment. Loss of information about correlations with the reservoir will introduce decoherence and noise to the system. In a similar way, the measurement process can be generalized by coupling the system to a second system that represents the detector [16].

In open quantum systems, the four dynamical equations discussed above are replaced by more general equations. The Schrödinger equation is replaced by the well-known master equation [17], while the Heisenberg equation of motion for operators turns into the quantum Langevin equation [14, 15], which typically takes the form

$$\partial_t \hat{A} = -\frac{i}{\hbar} [\hat{A}, \hat{H}] - \frac{i}{2\hbar} \{[\hat{B}, \hat{A}], \hat{F} - \gamma \partial_t \hat{B}\}, \quad (8)$$

where  $\{.,.\}$  denotes the anti-commutator,  $\hat{B}$  is the system operator that is involved in the coupling to the reservoir,  $\hat{F}$  is a noise operator, and  $\gamma$  a decoherence rate.

In phase space, the evolution of the Wigner function for open quantum systems leads generally to a strictly positive Wigner function [18, 19], thus introducing classicality [20]. Its dynamical equation takes the form of a Fokker-Planck equation [21, 22].

To our knowledge, the extension of the Moyal equation, i.e., the last of the four dynamical equations, has only been addressed in general terms by Ozorio de Almeida [23]. In this paper we aim to shed more light on this

case by studying the Moyal equation for a Schrödinger particle coupled to a thermal reservoir of harmonic oscillators. Our main result is that for Markovian reservoirs, in which correlations decay on a short time scale, the Moyal equation takes the form

$$\partial_t A(q, p, t) = \{A, H\}_M - 2\gamma p \frac{\delta A}{\delta F(t)} + F(t) \partial_p A, \quad (9)$$

where  $F(t)$  is a fluctuating force introduced by the reservoir, and  $\delta A/\delta F(t)$  denotes the functional derivative with respect to this force. The decoherence rate  $\gamma$  determines the time scale  $\gamma^{-1}$  on which information about reservoir correlations is lost.

## II. OPEN MOYAL EQUATION

To derive an example for an open Moyal equation, we consider the model proposed by Ford, Kac and Mazur [24, 25], in which a single, one-dimensional Schrödinger particle is coupled to a reservoir of  $N$  harmonic oscillators. The Weyl symbol of the Hamiltonian is given by [32]

$$H(q, p, q_n, p_n) = H_S + H_{\text{int}} + H_R \quad (10)$$

$$H_S = \frac{1}{2m} p^2 + V(q) \quad (11)$$

$$H_R + H_{\text{int}} = \sum_{n=1}^N \left( \frac{1}{2m_n} p_n^2 + \frac{1}{2} k_n (q_n - q)^2 \right), \quad (12)$$

with  $k_n = m_n \omega_n^2$ . Here  $q, p$  are position and momentum of the system particle, and  $q_n, p_n$  are the respective quantities for the  $n$ th reservoir oscillator. The symbol of  $H_R$  of the reservoir Hamiltonian alone can be found by setting  $q = 0$  in Eq. (12). Using the two different representations (5), (6) of the star product, the Moyal bracket can be written as

$$\{A, H\}_M = \frac{1}{i\hbar} (H(\mathcal{R}) - H(\mathcal{L})) A(q, p, q_n, p_n, t). \quad (13)$$

It therefore corresponds to linear differential operator on phase space that is defined through Eq. (13). It is shown in App. A that by a transformation

$$A(t) = e^{t\{\cdot, H_R\}_M} e^{qK(t)} \bar{A}(t), \quad (14)$$

the Moyal equation can be cast into the form

$$\partial_t \bar{A} = \{\bar{A}, H_S\}_M + \frac{p}{m} K(t) \bar{A} + F(t) \partial_p \bar{A}. \quad (15)$$

Here  $F(t)$  is a function of the reservoir's phase space variables  $q_n, p_n$  and  $K(t)$  is a differential operator acting on functions of the reservoir variables. Their definition is given in Eqs. (A15) and (A16), but for practical purposes only the relation

$$K(t)F(t') = -C(t - t') \quad (16)$$

$$C(t) = \sum_{n=1}^N k_n \cos(\omega_n t) \quad (17)$$

is relevant. The term proportional to  $F(t)$  in Eq. (15) could be introduced by modifying the system's potential energy as

$$V(q) \rightarrow V(q) - qF(t). \quad (18)$$

Therefore,  $F(t)$  can be interpreted as a time-dependent homogeneous force acting on the system. Because it depends on the reservoir variables, it will fluctuate with the state of the reservoir. We therefore can interpret  $F(t)$  as the phase-space symbol of a fluctuating random force. It is the equivalent of noise operators that appear in the quantum Langevin equation (8) and therefore may be called a noise (Weyl) symbol.

As  $K(t)$  corresponds to a derivative operator, it does not represent a phase space symbol, but rather a phase-space super-operator that maps the symbol of an operator to another symbol. We will see below that  $K(t)$  describes the dissipation in the system associated with the fluctuating random force.

The function  $C(t)$  of Eq. (17) can be interpreted as a force correlation function. It is shown in App. B that for a thermal reservoir of temperature  $T \gg \hbar\omega_n/k_B$  one has

$$\langle F(t)F(t') \rangle = k_B T C(t - t'). \quad (19)$$

## III. MARKOVIAN MOYAL EQUATION

In many cases of interest, the correlation function (17) decays on a time scale  $\tau$  that is much shorter than the time scales relevant for the evolution of the system. A physical example would be an atom as a system that is coupled to the quantized electromagnetic field as reservoir. This coupling is responsible for spontaneous decay of an excited atom, which for optical transitions happens on a time scale of nano seconds. The electromagnetic correlation function at these frequencies decays on the scale of femto seconds.

When the reservoir correlation function decays quickly, it is possible to make the Markov approximation. To analyze the Markov approximation in phase space, we first rewrite Eq. (15) as an integral equation,

$$\begin{aligned} \bar{A}(t) &= e^{t\{\cdot, H_S\}_M} \bar{A}(0) + \int_0^t dt' e^{(t-t')\{\cdot, H_S\}_M} \\ &\quad \times \left( \frac{p}{m} K(t') + F(t') \partial_p \right) \bar{A}(t'). \end{aligned} \quad (20)$$

We note that  $\bar{A}(t, q, p, q_n, p_n)$  is a function of both system and reservoir variables, while for a system operator the initial Weyl symbol  $\bar{A}(0, q, p)$  does not depend on the reservoir. By expanding Eq. (20) into a Dyson series one can see that  $\bar{A}(t)$  depends on  $F(t')$  through integrals of the form

$$I = \int_0^t dt' g(t') F(t'), \quad (21)$$

with  $g(t')$  being known functions, and convolutions of such integrals. The action of  $K(t)$  on such expressions amounts to

$$K(t)I = - \int_0^t dt' g(t') C(t-t'). \quad (22)$$

To perform the Markov approximation, we define the decay rate

$$\gamma = \frac{1}{m} \int_0^\infty dt C(t). \quad (23)$$

Then, for times  $t \gg \tau$ , we find

$$K(t)I = - \int_0^t dt'' g(t-t'') C(t'') \quad (24)$$

$$\approx -g(t) \int_0^t dt'' C(t'') \quad (25)$$

$$= -m\gamma g(t) \quad (26)$$

$$= -2m\gamma \frac{\delta I}{\delta F(t)}. \quad (27)$$

With this approximation [33], the open Moyal equation takes the form (9). In the following section we will verify this approximation at the example of a free particle.

#### IV. FREE PARTICLE COUPLED TO A RESERVOIR

To illustrate the general framework of the open Moyal equation we consider the situation in which the system particle is not subject to an external potential,  $V = 0$ . In this case the Markovian Moyal equation takes the simple form

$$\partial_t \bar{A} = \frac{p}{m} \partial_q \bar{A} - 2\gamma p \frac{\delta \bar{A}}{\delta F(t)} + F(t) \partial_p \bar{A}. \quad (28)$$

##### A. Canonical Weyl symbols

We first solve Eq. (28) for the canonical variables, where  $A(0) = q$  or  $A(0) = p$ , by making the ansatz

$$\bar{A}(q, p, t) = \beta_1(t)p + \beta_2(t)q + \beta_3(t), \quad (29)$$

where  $\beta_1, \beta_2$  are functions of time only while  $\beta_3(t) = \beta_3(t, q_n, p_n)$  may also depend on the phase-space variables of the reservoir. We use bold greek letters to indicate such a dependence. Inserting this into Eq. (28) and sorting the result with respect to  $q$  and  $p$  yields

$$\partial_t \beta_1 = \frac{1}{m} \beta_2 - 2\gamma \frac{\delta \beta_3}{\delta F(t)} \quad (30)$$

$$\partial_t \beta_2 = 0 \quad (31)$$

$$\partial_t \beta_3 = F(t) \beta_1, \quad (32)$$

so that  $\beta_2(t) = \beta_2(0)$  and

$$\beta_3(t) = \int_0^t dt' \beta_1(t') F(t'). \quad (33)$$

Inserting this into Eq. (30) yields

$$\partial_t \beta_1 = \frac{1}{m} \beta_2 - \gamma \beta_1, \quad (34)$$

which is solved by

$$\beta_1(t) = \beta_1(0) e^{-\gamma t} + \frac{\beta_2(0)}{m\gamma} (1 - e^{-\gamma t}). \quad (35)$$

For the symbols of position (momentum) we have  $\beta_1(0) = 0$  and  $\beta_2(0) = 1$  ( $\beta_1(0) = 1$  and  $\beta_2(0) = 0$ ), respectively, so that

$$\bar{A}_q(t) = q + \frac{p}{m\gamma} (1 - e^{-\gamma t}) + \frac{1}{m\gamma} \int_0^t dt' (1 - e^{-\gamma t'}) F(t') \quad (36)$$

$$\bar{A}_p(t) = e^{-\gamma t} p + \int_0^t dt' e^{-\gamma t'} F(t'). \quad (37)$$

Here we have adopted the notation that an index at the symbol of an operator refers to its initial value, e.g.,  $\bar{A}_q(0) = q$ . It remains to perform transformation (14). By using  $e^{L_R t} F(t') = F(t' - t)$  and approximation (27) we obtain

$$\begin{aligned} A_q(t) &= q e^{-\gamma t} + \frac{p}{m\gamma} (1 - e^{-\gamma t}) \\ &\quad + \frac{1}{m\gamma} \int_0^t dt' (1 - e^{-\gamma t'}) F(t' - t) \end{aligned} \quad (38)$$

$$A_p(t) = e^{-\gamma t} (p - m\gamma q) + \int_0^t dt' e^{-\gamma t'} F(t' - t). \quad (39)$$

We have verified that this solution agrees with the corresponding operator-valued solution of the quantum Langevin equation. Furthermore, it is shown in App. C that the Markovian solution presented here agrees with an exact treatment based on a specific correlation function  $C(t)$ .

To turn solutions (38) and (39) into symbols for the system particle alone, we have to take the average with respect to the reservoir. It is shown in App. B that for a thermal reservoir the mean noise force vanishes,  $\langle F(t) \rangle = 0$ . Therefore, the open Weyl symbols of position and momentum take the form (38) and (39) with  $F(t)$  set to zero.

The physical interpretation of this motion is as follows. The coupling to many oscillators with different frequencies results in a dissipation of energy from the particle into the reservoir. Therefore, the momentum of the particle is damped on a time scale  $\gamma^{-1}$ . The damping of the initial position  $q$  arises because in the model by Ford, Kac and Mazur all oscillators pull the system particle toward the common equilibrium point at  $q = 0$ . However,

the particle continues to move in its initial direction for a time of the order of  $\gamma^{-1}$ , which explains the term proportional to  $p/(m\gamma)$  in  $A_q(t)$ .

The reader may have noticed that  $A_p(0) = p - m\gamma q$  does apparently not fulfill the correct initial conditions. However, this is merely a consequence of the fact that the Markovian approximation is only valid for times  $t \gg \tau$ . The non-Markovian derivation in App. C shows that the term proportional to  $m\gamma q$  builds up on the short time scale  $\tau$  and then decays on the long time scale  $\gamma^{-1}$ .

## B. Variance Weyl symbols

To fully appreciate the influence of the reservoir one also needs to study the uncertainty of the canonical variables. We therefore consider symbols with initial condition  $\bar{A}(0) = q^2$  or  $\bar{A}(0) = p^2$  by making the ansatz

$$\bar{A} = \beta_1 p^2 + \beta_2 pq + \beta_3 q^2 + \beta_4 p + \beta_5 q + \beta_6. \quad (40)$$

As before, we sort the terms with respect to the power of  $q$  and  $p$ . For four of the six coefficients this can be done exactly as for the canonical symbols, leading to  $\beta_3(t) = \beta_3(0)$  and

$$\beta_2(t) = \frac{2\beta_3(0)}{m\gamma}(1 - e^{-\gamma t}) \quad (41)$$

$$\beta_5(t) = \int_0^t dt' \beta_2(t') F(t') \quad (42)$$

$$\beta_6(t) = \int_0^t dt' \beta_4(t') F(t'). \quad (43)$$

The remaining two coefficients obey

$$\partial_t \beta_1 = \frac{1}{m} \left( \beta_2 - 2\gamma \frac{\delta \beta_4}{\delta F(t)} \right) \quad (44)$$

$$\partial_t \beta_4 = 2\beta_1 F + \frac{1}{m} \left( \beta_5 - 2\gamma \frac{\delta \beta_6}{\delta F(t)} \right). \quad (45)$$

Using Eq. (43) leads to

$$\begin{aligned} \beta_4(t) &= 2 \int_0^t dt' e^{\gamma(t'-t)} \beta_1(t') F(t') \\ &+ \frac{1}{m} \int_0^t dt' \int_0^{t'} dt'' e^{\gamma(t'-t)} \beta_2(t'') F(t''). \end{aligned} \quad (46)$$

The functional derivative of  $\beta_4$  can then be simplified by noting that, for an arbitrary function  $g(t, t'')$ ,

$$\int_0^t dt' \int_0^{t'} dt'' g(t', t'') = \int_0^t dt'' \int_{t''}^t dt' g(t', t''), \quad (47)$$

to obtain

$$\partial_t \beta_1 = \frac{1}{m} \beta_2 - 2\gamma \beta_1, \quad (48)$$

which is solved by

$$\beta_1(t) = e^{-2\gamma t} \beta_1(0) + \frac{\beta_3(0)}{m^2 \gamma^2} (1 - e^{-\gamma t})^2. \quad (49)$$

Applying transformation (14) to Eq. (40) and using the expressions for  $\beta_i$  ( $i = 4, 5, 6$ ) yields

$$A(t) = \bar{A}(t) - m\gamma q(2(p - m\gamma q)\beta_1 + q\beta_2 + \beta_4), \quad (50)$$

where  $F(t')$  is replaced by  $F(t - t')$  everywhere.

Because  $\langle F(t) \rangle = 0$ , the averaged form of Eq. (50) takes the form

$$\begin{aligned} A(t) &= \beta_1 p^2 + q^2(\beta_3 - m\gamma \beta_2 + 2m^2 \gamma^2 \beta_1) \\ &+ pq(\beta_2 - 2m\gamma \beta_1) + \langle \beta_6(t) \rangle. \end{aligned} \quad (51)$$

The mean value of  $\beta_6$  can be evaluated using Eqs. (43), (46), and (19). Within the Markovian approximation, the result is given by

$$\langle \beta_6(t) \rangle = 2k_B T m\gamma \int_0^t dt' \beta_1(t') \quad (52)$$

$$\begin{aligned} &= mk_B T \left\{ \beta_1(0) (1 - e^{-2\gamma t}) \right. \\ &\quad \left. + \frac{\beta_3(0) (2\gamma t - e^{-2\gamma t} + 4e^{-\gamma t} - 3)}{\gamma^2 m^2} \right\}. \end{aligned} \quad (53)$$

It remains to apply the initial conditions,  $\beta_1(0) = 1$  for  $A_{p^2}(t)$  and  $\beta_3(0) = 1$  for  $A_{q^2}(t)$ , with all other coefficients being zero. Putting everything together we arrive at the open Weyl symbols

$$\begin{aligned} A_{q^2}(q, p, t) &= A_q^2 + q^2 (1 - e^{-\gamma t})^2 \\ &+ \frac{k_B T}{m\gamma^2} (2\gamma t - 3 - e^{-2\gamma t} + 4e^{-\gamma t}) \end{aligned} \quad (54)$$

$$A_{p^2}(q, p, t) = A_p^2 + mk_B T (1 - e^{-2\gamma t}) + e^{-2\gamma t} m^2 \gamma^2 q^2. \quad (55)$$

We have confirmed that this solution agrees with the operator-valued solution derived from the quantum Langevin equation. The physical interpretation is as follows. The term  $2k_B T t/(m\gamma)$  in  $A_{q^2}$  corresponds to a diffusion of the particle position. For solutions of the diffusion equation  $\partial_t f(t, q) = D \partial_q^2 f(t, q)$ , the variance of position increases as  $2Dt$  for sufficiently large times. This implies that the coupling to the reservoir can be linked to a diffusion coefficient  $D = k_B T/(m\gamma)$ . The Einstein-Smoluchowski relation  $D = \mu k_B T$  then implies that the mobility of the system particle is given by  $\mu = 1/(m\gamma)$ .

The term proportional to  $mk_B T$  in  $A_{p^2}$  describes the thermalization of the system particle through its coupling to the reservoir. Keeping in mind that  $\langle E_{\text{kin}} \rangle = \langle A_{p^2} \rangle/(2m)$  one can see that for times  $t \gg \gamma^{-1}$  the kinetic energy of the reservoir approaches  $k_B T/2$ , confirming the equipartition theorem. Finally, the terms proportional to  $q^2$  are a consequence of the dragging towards the origin in the Ford-Kac-Mazur model that we discussed above.

## V. DISCUSSION AND CONCLUSION

In the previous sections we derived the open Moyal equation (9), which describes the dynamics of open quantum systems coupled to a Markovian reservoir, and illustrated its features at the example of a free particle. The significance of the open Moyal equation is not so much in the specifics given here, but in the possibility to extend this model to describe open systems of larger interest.

This is the same situation as with master equation and quantum Langevin equation (8). Both equations have been derived from specific models, but have been generalized to describe the influence of various reservoir-induced effects on a large variety of systems. Examples include spontaneous emission, thermal excitation, spin dephasing, vibrational relaxation in molecules, and lossy optical cavities [14, 15].

In practice, most researchers do not derive reservoir properties from first principles but rather pick an ad hoc model to include the effect of a reservoir. This choice is not arbitrary but has to obey general principles. Positivity and trace preservation of the density matrix limit Markovian master equations to the celebrated Lindblad form [17]. Likewise, noise operators  $\hat{F}(t)$  and decoherence rate  $\gamma$  in quantum Langevin equations are related through a fluctuation dissipation theorem.

The same is true for the open Moyal equation. A rather trivial extension of the free particle discussed above is a particle under the influence of a constant external force  $F_0$ . This can be accomplished by including a linear potential  $V(q) = -qF_0$  in Eq. (A2). Using the techniques of Sec. IV it is not hard to see that the only change in solutions (38), (39) is then to replace  $F(t)$  by  $F(t) + F_0$ . The Weyl symbols of position and momentum are then modified according to

$$A_q(t) \rightarrow A_q(t) + \frac{F_0}{m\gamma} (t - \gamma^{-1}(1 - e^{-\gamma t})) \quad (56)$$

$$A_p(t) \rightarrow A_p(t) + \frac{F_0}{\gamma} (1 - e^{-\gamma t}). \quad (57)$$

For large time  $t$  this describes a particle moving with drift velocity  $F_0/(m\gamma)$ , which confirms the result for the mobility  $\mu$  found in Sec. IV B. Hence, the system's response to a linear perturbation is linked to the diffusion of  $q$  through the Einstein-Smoluchowski relation, which is one of the earliest examples of a fluctuation dissipation theorem.

The model presented here can be readily extended in several ways. An obvious extension is to combine the model by Ford, Kac and Mazur with more complicated external potentials  $V(q)$ . An interesting question arises for nonlinear potentials of Kerr type, where the exact solution for Weyl symbols exhibits a singularity [13]. Because dissipation often has a moderating effect, it may be possible that coupling to a reservoir may eliminate this singularity. One may also consider the effect of a reservoir on a system that consists of two or more inter-

acting particles, for instance for two photons interacting via cross Kerr modulation [26].

Another extension would be to generalize the quadratic coupling between the position of system and reservoir particles in the Ford-Kac-Mazur model. One way would be to introduce a distribution of equilibrium positions for the reservoir oscillators and to average over this distribution. This may eliminate the drag towards the origin that we discussed in Sec. IV. One may also introduce a different coupling like  $p \sum_n p_n$  in Eq. (12), which could be realized by a series of quantum LC circuits coupled through their mutual inductance [27]. In the context of quantum Langevin equations, it is possible to extend the interaction with a reservoir to nonlinear couplings [26, 28, 29], although this is considerably more involved. It is conceivable that the same could be accomplished for the open Moyal equation.

Finally one could follow the common practice in the field of quantum Langevin equations and simply pick an ad hoc model to obtain another open Moyal equation. This could be done by replacing  $p$  in Eq. (9) by another system observable  $O$ , and  $F(t)$  by random fluctuations of the corresponding time derivative  $\partial_t O$ . Given that phase space methods are an excellent tool to compare classical and quantum dynamics, and given that coupling a quantum system to a reservoir generally suppresses quantum correlations, the open Moyal equation may therefore provide a promising method to study how classical behaviour emerges in open quantum systems.

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## Appendix A: Derivation of the non-Markovian open Moyal equation

To avoid a cluttered notation, we will define linear operators  $L_i$  through

$$L_i A := \{A, H_i\}_M, \quad i = S, R, \text{int}. \quad (A1)$$

The explicit form of the Moyal bracket for the various parts of the Hamiltonian is then given by

$$L_S = \frac{p}{m} \partial_q + \frac{1}{i\hbar} [V(q - i\frac{\hbar}{2}\partial_p) - V(q + i\frac{\hbar}{2}\partial_p)] \quad (A2)$$

$$L_R + L_{\text{int}} = \sum_{n=1}^N \left[ \frac{p_n}{m_n} \partial_{q_n} - k_n (q_n - q) (\partial_{p_n} - \partial_p) \right]. \quad (A3)$$



To solve the reservoir part of Eq. (13), it is useful to switch to complex coordinates

$$\alpha_n = \frac{1}{\sqrt{2}} \left( \frac{q_n}{l_n} + i \frac{l_n}{\hbar} p_n \right) \quad (\text{A4})$$

$$l_n = \sqrt{\frac{\hbar}{m_n \omega_n}}, \quad (\text{A5})$$

which yields

$$\begin{aligned} L_{\text{int}} = & -q \partial_p \sum_{n=1}^N k_n + i q \sum_{n=1}^N \frac{k_n l_n}{\sqrt{2} \hbar} (\partial_{\alpha_n} - \partial_{\alpha_n^*}) \\ & + \partial_p \sum_{n=1}^N \frac{k_n l_n}{\sqrt{2}} (\alpha_n + \alpha_n^*) \end{aligned} \quad (\text{A6})$$

$$L_R = \sum_{n=1}^N i \omega_n (\alpha_n^* \partial_{\alpha_n^*} - \alpha_n \partial_{\alpha_n}). \quad (\text{A7})$$

We now go into an interaction picture with respect to the reservoir by setting

$$A(q, p, \alpha_n, \alpha_n^*) = e^{t L_R} \tilde{A}(q, p, \alpha_n, \alpha_n^*). \quad (\text{A8})$$

The Moyal equation then takes the form

$$\begin{aligned} \partial_t \tilde{A} = & e^{-t L_R} (L_S + L_{\text{int}}) e^{t L_R} \tilde{A} \\ = & L_S \tilde{A} - q \partial_p \sum_{n=1}^N k_n \tilde{A} + \sum_{n=1}^N \frac{k_n l_n}{\sqrt{2}} \\ & \times \left\{ \frac{i}{\hbar} q e^{-t L_R} (\partial_{\alpha_n} - \partial_{\alpha_n^*}) e^{t L_R} \right. \\ & \left. + e^{-t L_R} (\alpha_n + \alpha_n^*) e^{t L_R} \partial_p \right\} \tilde{A}. \end{aligned} \quad (\text{A9})$$

Operators of the form  $O(t) = e^{-t L_R} O(0) e^{t L_R}$  obey the differential equation  $\partial_t O = -[L_R, O]$ . It is not hard to see that for  $O(0) = \alpha_n$  and  $O(0) = \partial_{\alpha_n}$ , this equation has the solution

$$e^{-t L_R} \alpha_n e^{t L_R} = e^{i \omega_n t} \alpha_n \quad (\text{A11})$$

$$e^{-t L_R} \partial_{\alpha_n} e^{t L_R} = e^{-i \omega_n t} \partial_{\alpha_n}. \quad (\text{A12})$$

Hence the Moyal equation can be rewritten as

$$\begin{aligned} \partial_t \tilde{A} = & \left( L_S - q \partial_p \sum_{n=1}^N k_n \right) \tilde{A} + \sum_{n=1}^N \frac{k_n l_n}{\sqrt{2}} \\ & \times \left\{ \frac{i}{\hbar} q (e^{-i \omega_n t} \partial_{\alpha_n} - e^{i \omega_n t} \partial_{\alpha_n^*}) \right. \\ & \left. + (e^{i \omega_n t} \alpha_n + e^{-i \omega_n t} \alpha_n^*) \partial_p \right\} \tilde{A} \end{aligned} \quad (\text{A13})$$

$$= \{L_S - C(0) q \partial_p + \dot{K} q + F(t) \partial_p\} \tilde{A}, \quad (\text{A14})$$

with

$$F(t) = \sum_{n=1}^N \frac{k_n l_n}{\sqrt{2}} \{e^{i \omega_n t} \alpha_n + e^{-i \omega_n t} \alpha_n^*\} \quad (\text{A15})$$

$$K(t) = - \sum_{n=1}^N \frac{k_n l_n}{\sqrt{2} \hbar \omega_n} \{e^{-i \omega_n t} \partial_{\alpha_n} + e^{i \omega_n t} \partial_{\alpha_n^*}\} \quad (\text{A16})$$

To perform the Markovian approximation it is useful to reformulate Eq. (A14) by setting  $\tilde{A}(t) = \exp(q K(t)) \bar{A}(t)$ . Because  $[K(t), K(t')] = 0$  we can use the Baker-Campbell-Hausdorff formula and Eq. (16) to transform the open Moyal equation into

$$\begin{aligned} \partial_t \bar{A} = & \{e^{-q K(t)} L_S e^{q K(t)} - C(0) q \partial_p \\ & + e^{-q K(t)} F(t) e^{q K(t)} \partial_p\} \bar{A} \end{aligned} \quad (\text{A17})$$

$$= \{L_S + \frac{p}{m} K(t) - C(0) q \partial_p + (F(t) - q[K(t), F(t)]) \partial_p\} \bar{A} \quad (\text{A18})$$

$$= \{L_S + \frac{p}{m} K(t) + F(t) \partial_p\} \bar{A}, \quad (\text{A19})$$

which is Eq. (15).

## Appendix B: Averaging over the reservoir degrees of freedom

To obtain Weyl symbols that only depend on the system variables, one has to evaluate their mean value with respect to the reservoir degrees of freedom. Generally, the mean value of a symbol  $A(q, p)$  in phase space is expressed through

$$\langle A \rangle = \int dq dp A(q, p) W(q, p). \quad (\text{B1})$$

For a harmonic oscillator in thermal equilibrium, the Wigner function takes the form [30]

$$W = \frac{\omega}{2\pi \langle E \rangle} e^{-H(q, p)/\langle E \rangle} \quad (\text{B2})$$

$$= \frac{\omega}{2\pi \langle E \rangle} e^{-\hbar \omega |\alpha|^2 / \langle E \rangle} \quad (\text{B3})$$

with  $\langle E \rangle = \frac{1}{2} \hbar \omega \coth(\hbar \omega / (2 k_B T))$  the mean energy and  $H(q, p) = p^2 / (2m) + \frac{1}{2} m \omega^2 q^2$  the Weyl symbol of the Hamiltonian. This result can be derived using the thermal density matrix  $\rho = \exp[-\hat{H} / (k_B T)] / \text{Tr} \exp[-\hat{H} / (k_B T)]$  for the harmonic oscillator and Mehler's formula (see Sec. 10.13 of Ref. [31]). If we assume that the reservoir oscillators are thermalized, one can easily evaluate that  $\langle |\alpha_n|^2 \rangle = \langle E_n \rangle / (\hbar \omega_n)$  and  $\langle \alpha_n \rangle = \langle \alpha_n^2 \rangle = 0$ . Eq. (A15) then implies  $\langle F(t) \rangle = 0$  and

$$\langle F(t) F(t') \rangle = \sum_n k_n^2 l_n^2 \frac{\langle E_n \rangle}{\hbar \omega_n} \cos(\omega_n (t - t')). \quad (\text{B4})$$

For a hot reservoir, where  $\langle E_n \rangle \gg \hbar \omega_n$ , one has  $\langle E_n \rangle \approx k_B T$ , from which Eq. (19) follows.

## Appendix C: Solution for canonical observables without Markov approximation

In this section we repeat the calculations of Sec. IV A without making the Markov approximation (27). This

amounts to solving Eq. (28) with  $-2\gamma\delta\bar{A}/\delta F(t)$  replaced by  $K(t)\bar{A}/m$ . By making the same ansatz as in Sec. IV A we obtain the same equations and solutions for  $\beta_2$  and  $\beta_3$ , but  $\beta_1$  is determined by

$$m\dot{\beta}_1 = \beta_2 + K\beta_3. \quad (\text{C1})$$

Using Eq. (16) this can be transformed into

$$m\dot{\beta}_1 = \beta_2(0) - \int_0^t dt' \beta_1(t')C(t-t'). \quad (\text{C2})$$

This equation can be solved using a Laplace transformation  $g(t) \rightarrow \tilde{g}(s)$ ,

$$\tilde{\beta}_1(s) = \frac{1}{s + \frac{1}{m}\tilde{C}(s)} \left( \beta_1(0) + \frac{1}{ms}\beta_2(0) \right). \quad (\text{C3})$$

As an example for a reservoir memory function we consider [34]

$$C(t) = m\gamma\Gamma e^{-\Gamma t} \quad (\text{C4})$$

$$\tilde{C}(s) = \frac{m\gamma\Gamma}{s + \Gamma}, \quad (\text{C5})$$

which fulfills  $\int_0^\infty C(t)dt = m\gamma$ . The parameter  $\gamma$  should correspond to the decay rate associated with dissipation, while  $\tau = 1/\Gamma$  corresponds to the short time scale on which  $C(t)$  decays.

If  $s_i$  denotes the poles of  $\tilde{C}(s)$ , then the inverse Laplace transformation contains time-dependent exponentials  $e^{ts_i}$  multiplied by constant factors. For  $\Gamma \gg \gamma$ , we can make a separate Taylor expansion of the poles in the exponent and the constant terms around  $\Gamma = \infty$ . The poles  $s_i$  are then approximately given by  $-\gamma$  and  $-\Gamma$ . After applying transformation (14) we obtain, to leading order in  $1/\Gamma$ ,  $A_q(t)$  of Eq. (38) as well as

$$A_p = e^{-\gamma t}p - m\gamma q(e^{-\gamma t} - e^{-\Gamma t}) + \int_0^t dt' e^{-\gamma t'} F(t-t'). \quad (\text{C6})$$

For times  $t \gg \tau$  this solution agrees with the Markovian result (39). It only differs by the short-living term proportional to  $e^{-\Gamma t}$ , which ensures that the correct initial conditions are fulfilled.

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  - [32] The Hamiltonian operator takes the same form, with the symbols  $q, p, q_n, p_n$  replaced by the respective operators because  $S[g(\hat{q})] = g(q)$  for any operator  $g(\hat{q})$  that is a function of  $q$  only. A similar statement holds for operators of the form  $g(\hat{p})$ .
  - [33] While  $\delta I/\delta F(t') = g(t')$  for all points  $0 < t' < t$ , one has to be careful at the boundary of the integral  $I$ . The factor of 2 in Eq. (27) is a consequence of the following procedure. We rewrite  $I$  by replacing the integration boundary  $t$  by  $\infty$  and the function  $g(t')$  by  $g(t')\theta(t-t')$ , with  $\theta$  the step function. Then  $\delta I/\delta F(t) = g(t)\theta(0)$ . Setting  $\theta(0) = 1/2$  yields Eq. (27).
  - [34] Eq. (17) suggests that  $\partial_t C(0) = 0$ . Although example (C4) does not obey this relation, we have verified that in the limit  $\Gamma \gg \gamma$  it yields the same result as more complicated examples that do fulfill it.